Charge Density Study of a Pentapeptide

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The largest molecule examined under our X-ray charge density analysis was the pentapeptide Boc-Gln-D-Iva-Hyp-Ala-Phol(Boc=butyloxycarbonyl, Iva=isovaline=ethylalanine, Phol=phenylalaninol) (**Figure 1**) for which 217226 reflections were measured to give 17144 unique reflections. The large redundancy makes it possible to identify outlier measurements (if present) and to obtain highly accurate average values. Of particular interest is comparison of charges in the peptide bond atoms along the polymer chain. Results from the topological analysis of the electron density are given in **Table 1**. Most striking is the consistency of the topological results, the only outlier being the side-chain nitrogen, which is expected to differ. For comparison, analysis of theoretical results are presented. However, for this large molecule a 6-31G** basis set had to be used, which may not be sufficiently accurate for the current purpose. The isolated molecule calculation also neglects the effect of the crystalline matrix.

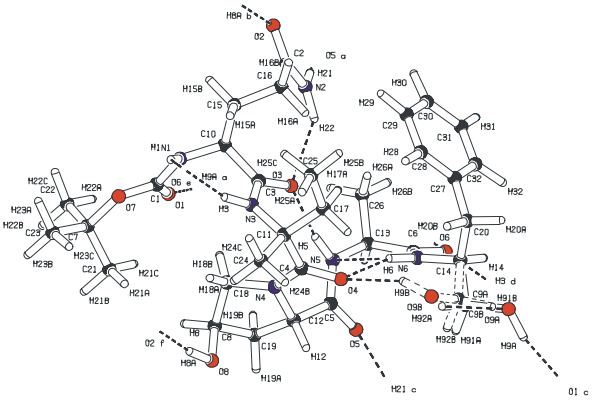

Figure 1. Molecular structure of the polypeptide Boc-Gln-D-Iva-Hyp-Ala-Phol.

Table 1. Net charges of the nitrogen atoms in the polypeptide Boc-Gln-D-Iva-Hyp-Ala-Phol

	Experiment	Theory (B3LYP/6-31G**)
	Topological integration of the experimental density	Topological integration of the theoretical density
N1	-0.77	-1.20
N2*	-1.02	-1.29
N3	-0.71	-1.24
N4	-0.85	-1.19
N5	-0.71	-1.28
N6	-0.88	-1.28

* nitrogen atom in the glutamine side-chain

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